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Probabilistic Characterization of the Inner Order of Random Structures

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The classical stereological quantities N_V, L_V, S_V, V_V and others are mean values not giving an insight in the dependencies, orientations and further kinds of the inner structure. To describe and analyse the inner order the covariance, the reduced second moment function (K-function), the pair distribution function (pair correlation function), the radial distribution function, the integrated radial distribution function, and the second-order product density are defined and interpreted. The stereological determination of the pair distribution function for point and fibre systems is demonstrated. Information on a suitable software-package is given.

INTRODUCTION

To quantify and anlyse correlations, clustering, attraction, repulsion of the elements within random structures such as point processes, fibre, surface, and volume processes some quantities and functions are useful: covariance, K-function, pair distribution or pair correlation function, radial distribution function, integrated radial distribution function, second order density function, and others. Some of them have been introduced and used in specific scientific areas over years. For example, the radial distribution function is in use in solid state physics with X-ray scattering technique.

In last years such characteristics have been introduced in stereology with applications in material and life science. Formulas, equations, estimators have been given to compute them from planar and thin sections of the structures under study. Computer software for them is available. Furthermore, they are mathematically rigorous defined, studied, and in part generalized to other cases such as anisotropic structures.

HEURISTICAL APPROACH

For any random structure ϕ, in particular in three dimensions, the covariance $\mathrm{cov}(\phi(V_1), \phi(V_2))$ is, of course, a suitable measure for possible correlations. Here V_1 and V_2 denote two volumina in the three dimensional space and the random variables $\phi(V_1)$ and $\phi(V_2)$ are the random number of points in V_1 and V_2, respectively, if ϕ is a random point structure, the random total fibre lengths in V_1 and V_2 in case ϕ is a random

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fibrous structure, and analoguously for random surface and body systems, respectively. But under certain conditions there exist real-valued functions only of one real variable which are simpler to handle with, and giving complete or nearly complete insight in the inner order of the structure.

Let be given a spatial point structure, randomly positioned, denoted by ϕ, and assumed to be homogeneous and isotropic. An intuitive approach to the pair distribution function is the following. Consider two infinitesimal small spheres ΔV_1 and ΔV_2 the centres of which have a distance r. Then $\phi(\Delta V_1)$ and

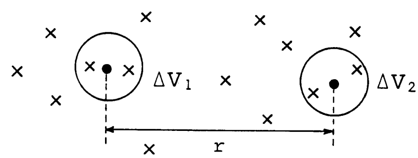

Fig. 1. Random point structure with samll spheres:

$\phi(\Delta V_2)$ are the random numbers of points in ΔV_1, ΔV_2, respectively. Because ϕ is homogeneous for the mathematical expectation $E\phi(\Delta V_i) = N_V \cdot \Delta V_i$, i=1,2, holds, where N_V is the volume density of ϕ, i.e. the mean number of points in the unit cube. Then we consider the ratio

$$\frac{E(\phi(\Delta V_1)\cdot\phi(\Delta V_2))}{E(\phi(\Delta V_1))\cdot E(\phi(\Delta V_2))} = \frac{E(\phi(\Delta V_1)\cdot\phi(\Delta V_2))}{N_N^2\cdot\Delta V_1\cdot\Delta V_2} = g_V(r) \qquad (1)$$

Because of the assumptions the ratio is only a function of the distance r and is denoted by $g_V(r)$. It is said to be the pair distribution function of ϕ (because we considered a pair of spheres and centres, respectively!).

If the random numbers $\phi(\Delta V_1)$ and $\phi(\Delta V_2)$ are independent then we have

$$E(\phi(\Delta V_1)\cdot\phi(\Delta V_2)) = E(\phi(\Delta V_1)\cdot E(\phi(\Delta V_2))) \qquad (2)$$

and consequently $g_V(r)=1$ for all $r \geqq 0$. Thus for a homogeneous spatial Poisson point process we have a pair distribution function constantly equal to one. In general, $g_V(r)$ is a non linear function of r, and values of the pair distribution function greater than one indicate attraction of possible particles at the points, while values of the pair distribution function smaller than one indicate repulsion. Peaks of the function reflect preferred distances between the points, and minima give rarely occuring distances. As r tends to zero then the pair distribution function converges to a value c, $0 \leqq c \leqq \infty$. As r tends to infinity then the pair distribution function under weak assumptions tends to one, and the rate of convergence gives information on the degree of randomness of the given point structure in comparison with the complete randomness of the Poisson point structure.

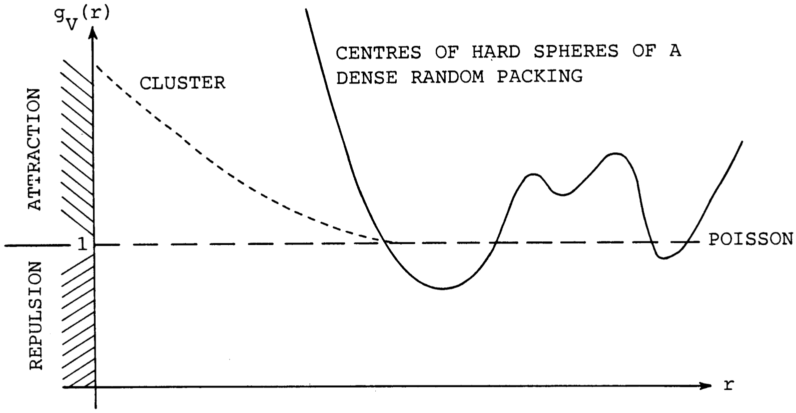

Fig. 2. Examples of the pair distribution function

STRONG DEFINITIONS

Let $\mathcal{B}^3$ be the σ-field of Borel sets of the three-dimensional Euclidean space, and N is the space of all locally finite counting measures φ on R^3. $\mathcal{N}$ is the minimal σ-field of subsets on N which makes the function $\varphi \rightarrow \varphi(B)$ measurable for all bounded $B \in \mathcal{B}^3$. A random point process ϕ is a probability space $[N, \mathcal{N}, P]$ with the probability distribution P on $\mathcal{N}$. Thus, for a subset $B \in \mathcal{B}^3$, $\phi(B)$ is the random number of points of ϕ in B, and $P(\phi(B)=k)$ is the probability that there are k points of ϕ in B.

The measure $\mathcal{C}_P^!$ on the product σ-field $\mathcal{B}^3 \otimes \mathcal{N}$ defined by

$$\mathcal{C}_P^! (B \times Y) = \int_N \int_B 1_Y (\varphi - \delta_x) \varphi(dx) P(d\varphi), \quad B \in \mathcal{B}^3, \; Y \in \mathcal{N}, \tag{3}$$

is said to be the reduced Campbell measure of or ϕ or P, respectively. Here δ_x equals one for $x \in Y$, and zero otherwise.

For Y=N the reduced Campbell measure gives a new measure on $\mathcal{B}^3$:

$$\Lambda_P(B) = \mathcal{C}_P^!(B \times Y) = \int_N \varphi(B) P(d\varphi), \quad B \in \mathcal{B}^3. \tag{4}$$

Λ_P is called the intensity measure of P. Obviously is $\Lambda_P(B) = E\,\phi(B)$. In case ϕ is the non-homogeneous Poisson point process then the intensity measure is well-known. If ϕ is stationary (homogeneous), i.e. invariant with respect to translations, then it is

$$\Lambda_P(B) = \lambda_P \cdot \nu(B), \quad B \in \mathcal{B}^3, \tag{5}$$

where ν is the Lebesgue measure on $\mathcal{B}^3$ and λ_P is a constant, called the intensity of ϕ. It is

$$\lambda_P = \Lambda_P([0,1]^3) = E\,\phi([0,1]^3), \tag{6}$$

in other words λ_P equals N_V which is the common notation in stereology. If for a not necessarily stationary point process the intensity measure is σ-finite then for Λ_P-almost all $x \in R^3$ there exist unique probability distributions $P_x^!$ on $\mathcal{N}$ with

$$\mathcal{C}_P^!(B \times Y) = \int_B P_x^!(Y)\ \Lambda_P(dx),\ B \in \mathcal{B}^3,\ Y \in \mathcal{N}. \tag{7}$$

The distribution $P_x^!$ is said to be the reduced Palm distribution of the random point process with respect to the point x. It is a generalization of the Palm-Khintchine function for stationary point processes on R^1 and can be interpreted as the conditional probability distribution of the point process under the condition that at x there is a point of the point process (which condition has the probability zero; therefore the relatively complicated definition of the reduced Palm distribution is necessary). The point x by itself is not counted in the event Y.

Now, let us assume that the random point process ϕ is stationary and isotropic, i.e. invariant under translations and rotations. The function $K_V(r)$ defined by

$$K_V(r) = \frac{1}{\lambda_P} \int_N \varphi(b(0,r))\,P_0^!(d\varphi) \tag{8}$$

is said to be the reduced second moment function, in short also K-function. Here b(0,r) is a sphere with the origin 0 of R^3 as centre and radius r. With the help of the interpretation of $P_x^!$ it is obvious that $\lambda_P \cdot K(r)$ can be interpreted as the mean number of points in a sphere with radius r centred at the origin 0 under the condition that at 0 there is a point of the point process, which is not counted in $\varphi(b(0,r))$. The K-function is analytically well-known for important models of point structures.

Then the pair distribution function (or pair correlation function) is defined by the first derivative of the reduced second moment function, in case it exists:

$$g_V(r) = \frac{1}{4\pi r^2}\,\frac{dK_V(r)}{dr},\ r \geq 0. \tag{9}$$

Although it is called pair 'distribution function' it is, of course, not a distribution function in the usual sense of probability theory; more likely it is a density function.

The second-order product density (also named second order density function)

$$\rho_V(r) = \lambda_P^2\, g_V(r), \tag{10}$$

the radial distribution function

$$R(r) = \lambda_P \cdot 4\pi r^2\, g_V(r), \tag{11}$$

and the integrated radial distribution function

$$\mathcal{G}(r) = \lambda_P \int_0^r R(x)\,dx \tag{12}$$

are also in use.

Edge-corrected unbiased estimators of the K-function have been constructed and studied by Ripley, Ohser, Ohser & Stoyan, see also Diggle (1983). To estimate the pair distribution function one can use general density estimators, published for example by Jolivet.

STEREOLOGY FOR THE PAIR DISTRIBUTION FUNCTION OF A POINT STRUCTURE

We consider centres x_n of random spheres with independent identically distributed radii $r_{V,n}$ with distribution function R_V which are assumed to be independent on the randomly positioned centres x_n. Denote by g_V the pair distribution function of the point structure of the x_n which is assumed to be homogeneous and isotropic. We'ld like to estimate g_V using information of a planar section, see also König et al (1983). In the section plane there is observed a random structure of circles with centres y_n and random radii $r_{A,n}$ with distribution function R_A and pair distribution function g_A for the y_n. Then the pair distribution function g_V is a solution of the integral equation

$$g_A(r) = \frac{1}{2R^2} \, , \int_0^{2R} (2R-x)\, g_V(\sqrt{r^2+x^2})\, dx \tag{13}$$

in case of constant radii $r_{V,n} = R$, and of the integral equation

$$g_V(r) = \frac{b^2}{2} \int_0^{\infty} (x + \frac{1}{b}) \exp(-bx)\, g_V(\sqrt{r^2+x^2})\, dx \tag{14}$$

in case of exponentially distributed (with parameter b) radii $r_{V,n}$, see Hanisch & Stoyan (1981), Hanisch (1983), König & Stoyan (1986). For an arbitrary distribution function R_V the integral equation for g_V is given in Hanisch (1983) see also König & Stoyan (1986), where one can find also analytical methods for solving the integral equations. In practical applications R_V in general is unknown. Therefore another integral equation has been given and analytical procedurs have been discussed to get g_V without using R_V but only quantities of the section plane, see König & Stoyan (1986).

The stereological determination of an estimator of the pair distribution function g_V of the centres of sinter metall spheres by a planar section of a sample of sinter metall is published in Hanisch et al. (1985) while a discussion of this example for a thin section of the sphere system can be found in König & Stoyan (1986).

Integral equations for the pair distribution function g_V of centres of arbitrary convex isotropic particles instead of spheres can be derived analoguously. It is our conjecture that in most cases these integral equations are quite "close" to those for g_V in the case of spheres.

On the other side only linear sections of the spheres might be given. Denoting by g_L the pair distribution function of the squared half on the intersection chords the following integral equation for g_V holds

$$g_L(r) = \int_0^\infty \int_0^\infty h_L(u,v)\, g_V(\sqrt{r^2+u^2+v^2})\, du\, dv, \qquad (15)$$

where $h_L(u,v)$ depends on the distribution function of the half intersection chord lengths.

Finally, there is also a relationship between the scattering analysis of a random point structure and the pair distribution function. If one considers the scattering of X-rays by matter as in solid state physics or materials science then one gets the following equation in the case of a stationary and isotropic spatial point process with intensity λ

$$g_V(r) \approx 1 + \frac{1}{2\pi^2 \lambda_r} \int_0^\infty h(I(h)-1)\sin(hr)\, dh, \qquad (16)$$

where $I(h)$ is the scattering intensity function describing the distance proportions between the atoms, and $h=\|\underline{h}\|$ with $\underline{h}=(h_1, h_2, h_3)$ being the scattering vector. Thus, the pair distribution function and the intensity function are related to each other by Fourier transform. If, for example, the stationary Poisson process is given, then $g_V(r)\equiv 1$ and $I(h)\approx 1$.

Also the orientation analysis of planar point structures can be done with the help of a generalized K-function which depends on r and an angle, suitable defined distrubution functions for the orientations and by the rose of orientations, see for example, Ohser & Stoyan (1981). That means that the K-function can also be used to quantify the degree of anisotropy in the case of anisotropic point patterns and the detection of inner orientations in the point pattern in the case of isotropy if, for example, the points are positionned on an isotropic system of random fibres.

A SOFTWARE - PACKAGE

For practical use in particular in materials science we have developped a software-package, named AMBA/R-TECH, for the image processing system A6471 produced by the company "ROBOTORON" (G.D.R.). It has the following programs for the second order analysis of point structures:

- PDF It computes unbiased estimators $\hat{g}_A$ of the pair distribution function of planar point systems (for example obtained by sectioning)
- STEREO A Program to get the pair distribution function g_V for the three-dimensional point structure by solving the suitable integral equation, if g_A for the plane is given.
- REDU To get estimators for the reduced second moment function $K(r)$
- COV 1,2,3 Different estimators for the covariance based upon Poisson point processes, lattice processes and further test systems, respectively
- ORIENT Orientation analysis of planar point structures with the help of edge-corrected estimators, based upon the generalized reduced second moment function.

These programs have been used for applications in materials and life science and the results are very good.

PAIR DISTRIBUTION FUNCTION AND ITS STEREOLOGY FOR SPATIAL FIBRE STRUCTURES

Let F be a random fibrous structure as, for example, fibres in glass, paper and further material, dislocation lines in crystalline matter before and after hot-compression, nerves, central lines of capillaries. Mathematically, we consider a random fibre system to be a random one-dimensional closed set in the three-dimensional space. Then F can be described by a uniquely determined random measure ϕ. For a subset $B \subsetneq R^3$ the random variable $\phi(B)$ is the random total length of fibre pieces of F contained in B. We assume stationarity and isotropy and consider two infinitesimal small volumina ΔV_1 and ΔV_2 with the random total fibre lengths $\phi(\Delta V_1)$ and $\phi(\Delta V_2)$ of F in these volumina, see Fig. 3.

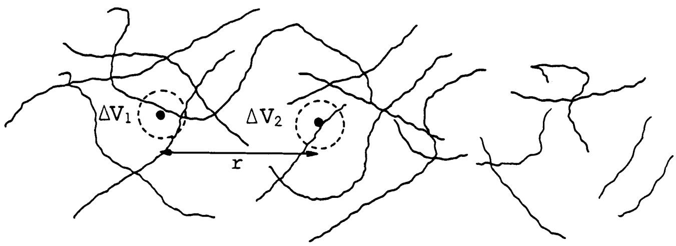

Fig. 3. Random fibre structure with small volumina

Then the ratio (1) is the pair distribution function $g_V(r)$ of the random fibre structure F. In a strong definition it can be given analoguously to formula (9) by

$$g_V(r) = C \cdot \frac{dK(r)}{dr} \tag{17}$$

where K(r) is a suitable defined reduced second moment function. Not going into mathematical details we can interpret $L_V K(r)$ as the mean total length of the fibre pieces in a sphere b(x,r) where x is a randomly chosen fibre point and L_V is the mean total length of the fibre pieces per unit volume, i.e. the length density in space.

The stereological problem is to estimate g_V for the spatial random fibre structure using only quantities of planar or thin section of the fibre system F. A procedure for planar section has been given in Hanisch et al (1985) where also a sample of capillaries in human brain is studied. Different estimators in the case of planar and thin sections can also be found in König & Stoyan (1986).

For an object volume V of a crystal foile with thickness d and an arbitrarily chosen projection plane which can be realized, for example, by transmission electron microscope images we'ld like to get the pair distribution function $g_V(r)$ of a three-dimensional dislocation configuration in crystals via the pair distribution function $g_A(r)$ of the fibre projection lines (which is a stationary and isotropic random fibre system in the two-dimensional space, i.e. the plane) on projection plane.

Then the pair distribution function $g_V(r)$ is approximately (namely under the condition that the directions of the fibres in two arbitrary points of the fibre system are independent) given by the following integral equation

$$g_A(r) = \frac{2}{d^2} \int_0^d (d-x) g_V(\sqrt{r^2+x^2})\,dx , \tag{18}$$

where x is a coordinate perpendicular to the foil plane. To solve this equation one needs an estimator for g_A, see Stoyan (1981) and König & Stoyan (1986) where different methods have been given. The difficulty is that the point system of intersection points of a fibre system in the plane does not contain sufficient information to determine the pair distribution function. Either approximations are possible for not too small r or in addition to the intersection points the angles under which the fibres intersect the plane of intersection have to be measured, see König & Stoyan (1986). In that case exact solutions are possible.

The orientation analysis and the scattering analysis of systems of fibres are possible too but need more detailed study than in the case of point processes.

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